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Title: From Spline Smoothing to Quantum Information and Beyond

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From Spline Smoothing to Quantum Information and Beyond

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Nuclear Material Control & Accountability (SAFE-4)

4 - 6 June 2014

Abstract

A view of Professor Grace Wahba as a PhD advisor and colleague from her PhD graduate student James Wendelberger. He describes early PhD thesis work and progresses through later work throughout his career. From ideas and work on multidimensional smoothing splines the description progresses and expands to diverse application areas in industry, government and academia. It moves to the field of nanoscience, touches on the Higgs Boson, and on to characterizing the variability of inventory differences associated with radionuclide measurements. It supports the notion that Professor Wahba provided an infectious curiosity with a deep understanding of the theoretical and practical aspects of problems while infusing a mathematical and scientific rigor to applied problems of practical significance.

Motivation and Direction

- Radiology cobalt-60 scattering radiation distribution
- Hilbert space
- Sobolev space
- Know where your estimator is coming from!
- 2m-2k-d > 0
- Dilogarithms splines on the sphere - Dick Askey
- Computer code – Jay Fleisher, Bill Fortney
- Get off the grid!

Smoothing Spline: A Special Case

- Thin plate analogy to Schrödinger equation and Hamiltonian(s)
  - Schrödinger – evolution in time
  - Hamiltonian – forces and energy
    - Kinetic energy – =0
    - Potential energy
      - Spring energy deviations
      - Deformed plate Integral

Grand Advisors of Grace Wahba

- Emanual Parzen
- Michel Loève
- Paul Pierre Lévy
- Jacques Salomon Hadamard
- C. Émile (Charles) Picard
- Gaston Darboux
- Michel Chasles
- Simeon Denis Poisson
- Advisor 1: Joseph Louis **Lagrange**
  Advisor 2: Pierre-Simon **Laplace**

… Gregory Palamas – 1363 ish

Collaborators

- Meteorology – Professor Don Johnson +
- Ground water – Professor Mac Barthow +
- Smoothing Spline Algorithm - Gene Golub
- Spline on Sphere Algorithm - Dick Askey

Attributes

- Most patient advisor
- Always trying to find strengths in her students

Career

- In the Academic World
  - UW Space Science and Engineering Postdoc
  - Oakland University
  - University of New Mexico - Los Alamos
  - University of New Mexico - Albuquerque
- Out of the Academic World
  - General Motors Research Laboratory
  - Urban Science Applications Inc.
  - Nano Stat LLC
  - Guest Scientist
  - Scientist Los Alamos National Laboratory
- References
  - GMR
  - PStat
  - UNM Graduate Student Reference
  - LANL Reference

The Guiding Light

$$\hat{f} = \underset{f \in \mathcal{H}_m^d}{\operatorname{argmin}} \left[\frac{1}{N} ||\mathcal{L}f - z||_2^2 + \lambda \int_{\mathcal{R}^d} \nabla^{(2m)} f \right]$$

Lagrange multiplier λ,

Laplacian $\Delta = \nabla^2$ (divergence $\nabla\cdot$ of gradient ∇)

and, of course, a

Hilbert Space $\mathcal{H}_m^d$.

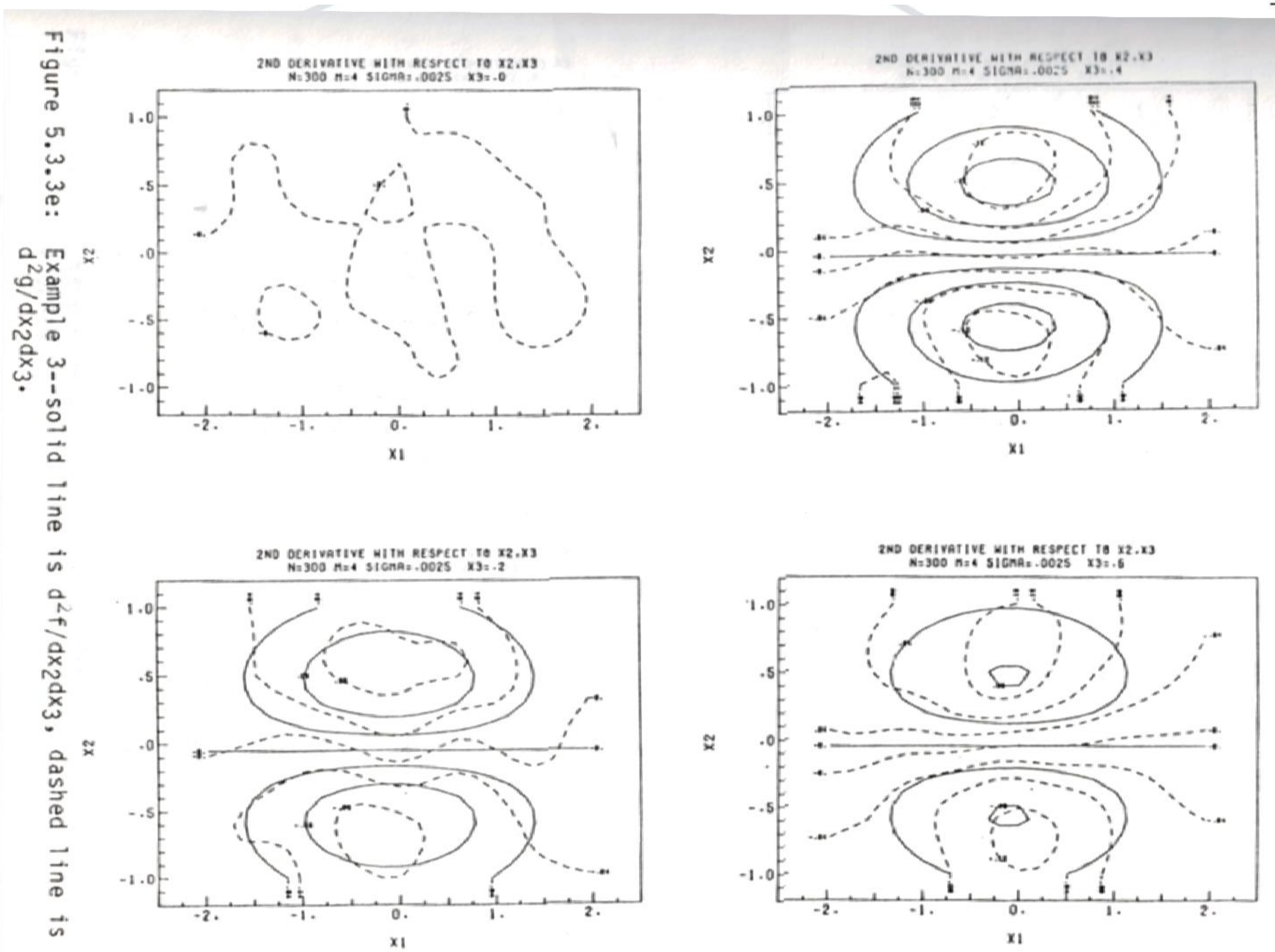
And how do I know what this means?

an estimate of a function,
an operator "argmin",
a function "f",
a set operation "$\in$",
a set of functions "$\mathcal{H}_m^d$",
a norm,
a square of a scalar,
scalars d, m, N and λ (a Greek letter),
a vector of N linear functionals "$\mathcal{L}$",
a vector of scalars,
a Laplacian operator ∇^2 (a not so well known symbol),
a d-dimensional integral (a better known symbol)
and a set of d-dimensional points "$\mathcal{R}^d$".

Context!

- Null space
- Interpolation limit
- Polynomial regression limit
- And it would also be nice to know 2m-2k-d>0

Derivative Estimation 2m-2k-d > 0



Hilbert Space?

- A set of objects
- With an inner product
- It is complete

Really? That simple?

"What does this have to do with statistics?"

The Laplacian Smoothing Spline

- Irregularly spaced points
- Multiple dimensions
- Smoothness
- Computer Code
  - First
  - Fortran
  - QR and SVD
  - Reuse

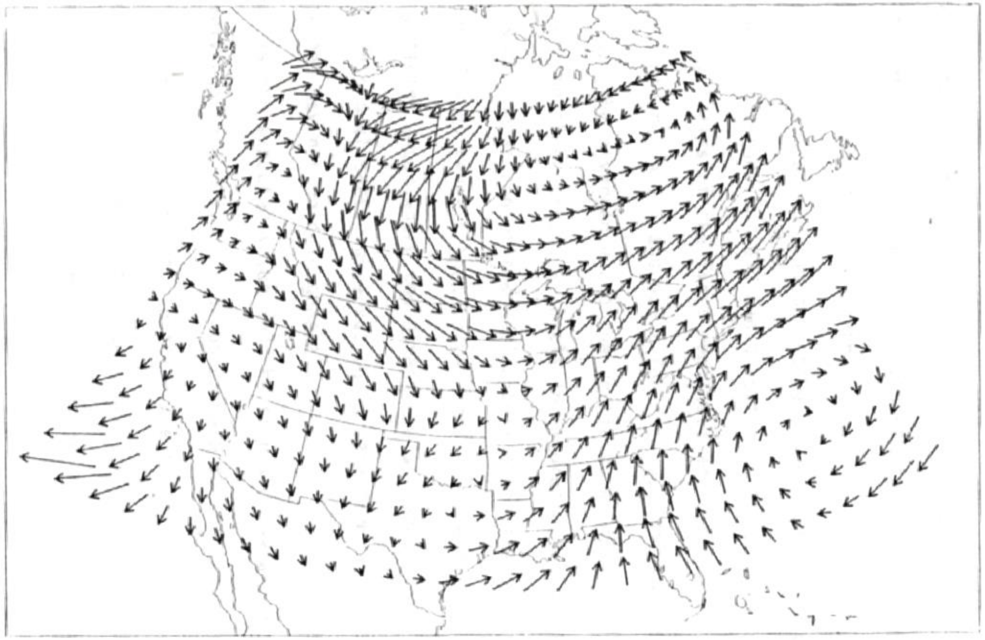
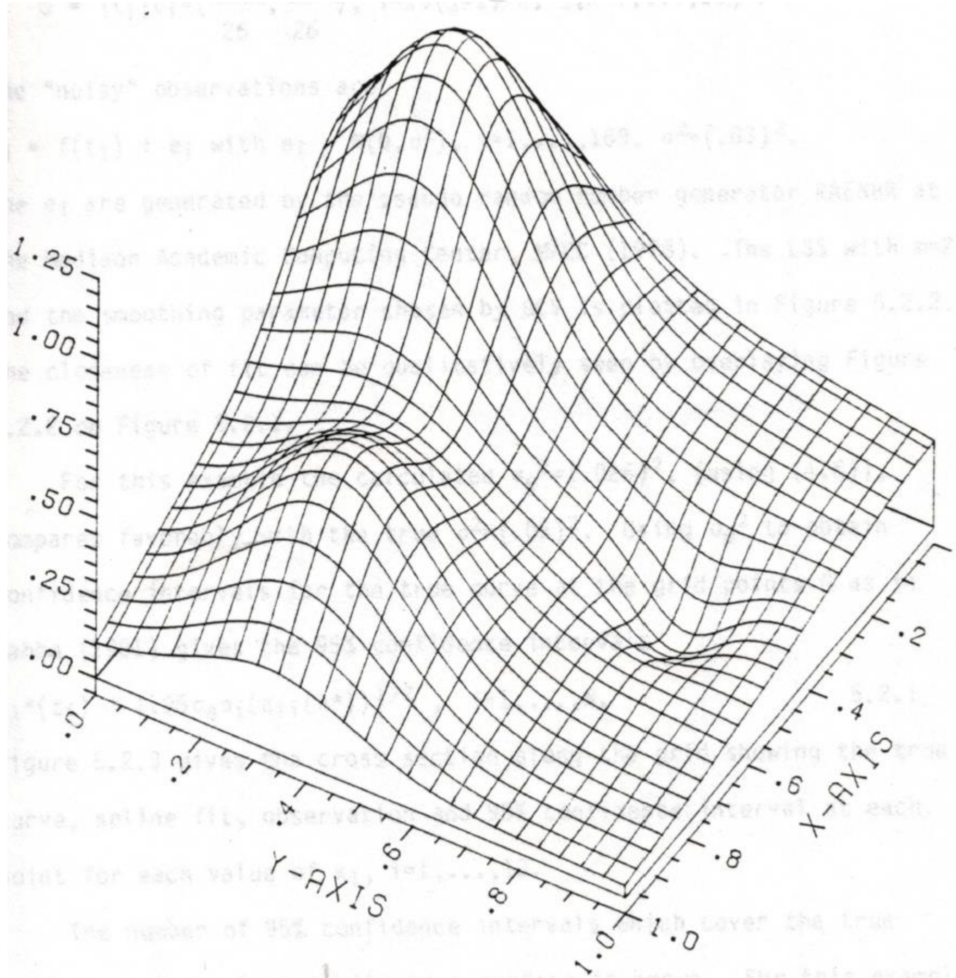


Figure 6.4.4c: The 850 mb Pressure Level Replicate 1 Objectively Analyzed Field on a 2 by 2 degree Grid (.6 m/s).

Test Function

- Franke's principal test function
- ~400 pages



Meteorology

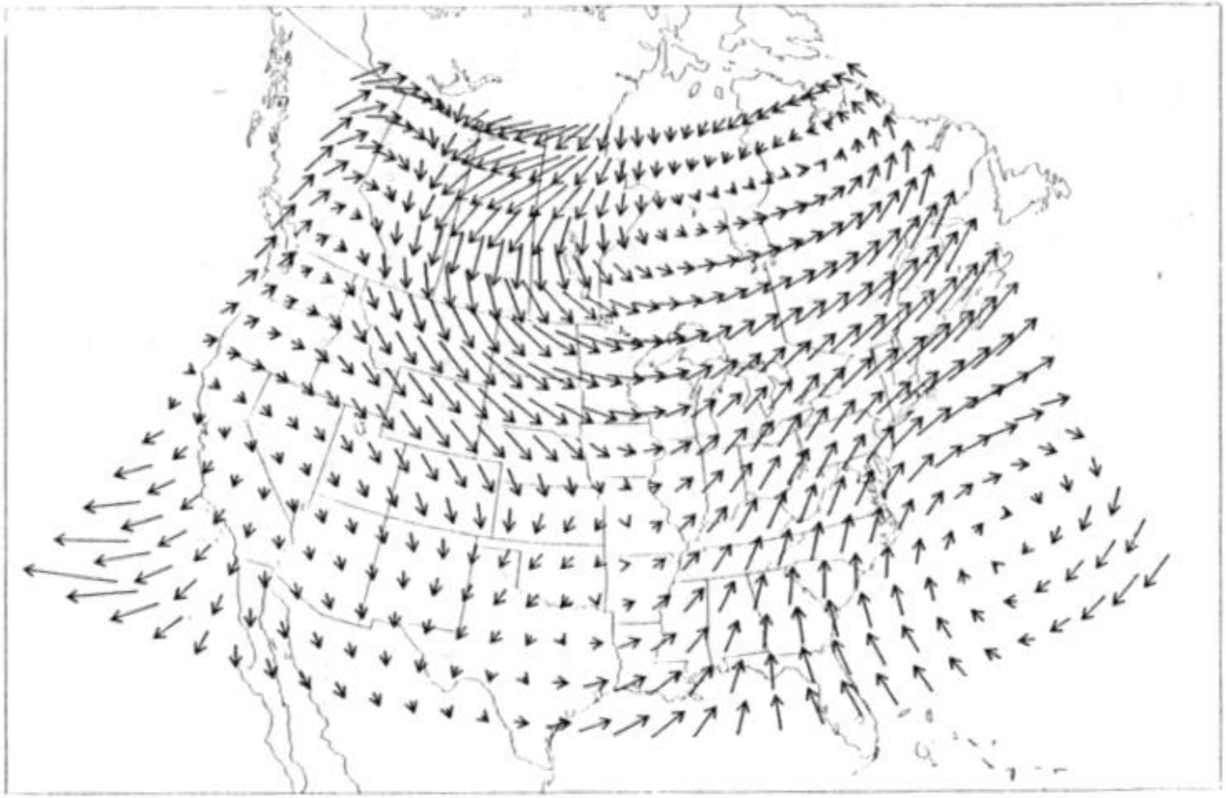


Figure 6.4.4c: The 850 mb Pressure Level Replicate 1 Objectively Analyzed Field on a 2 by 2 degree Grid (.6 m/s).

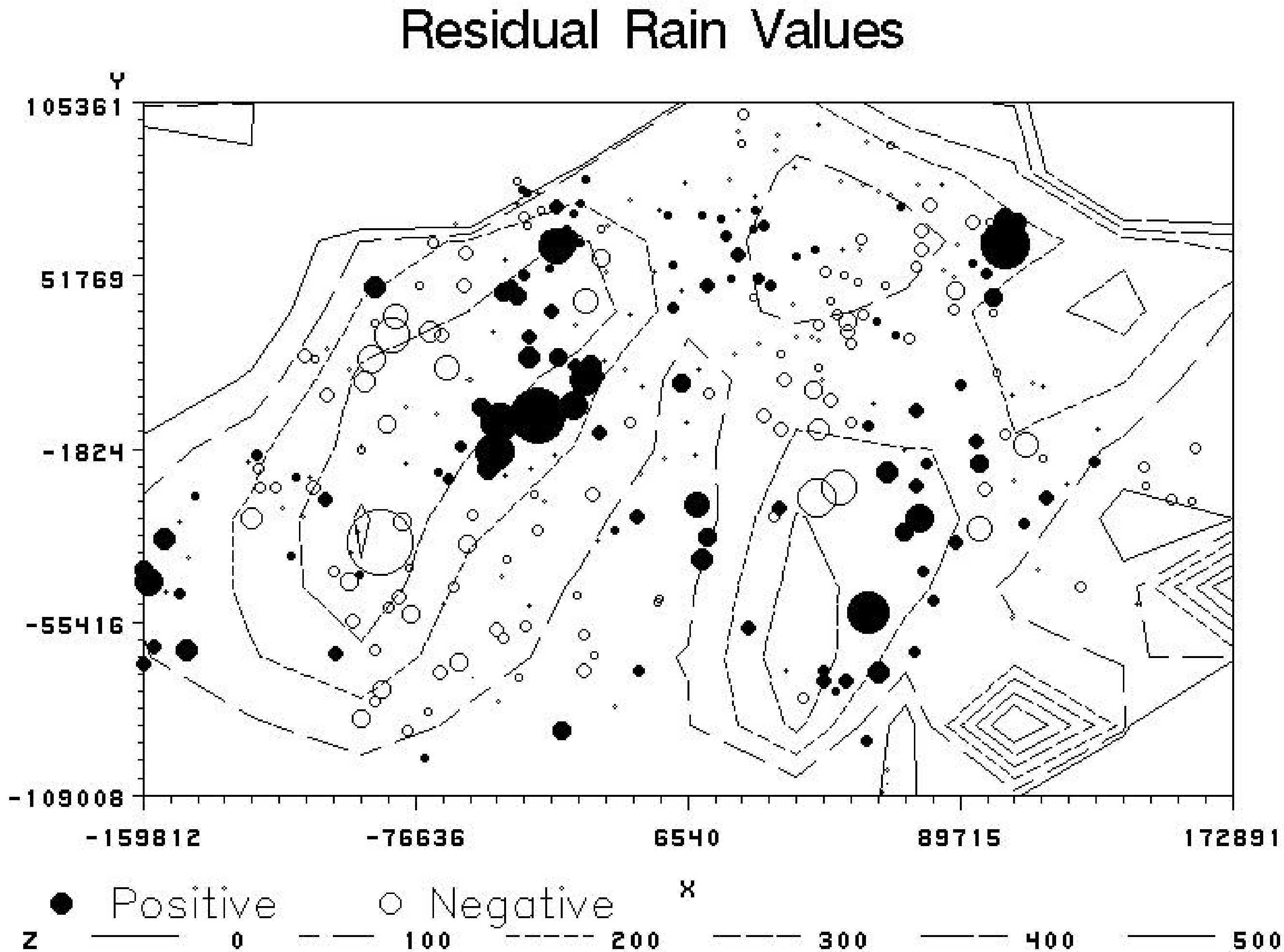
Ground Water Concentrations

- Ground water
  - Time series d=4
  - Dimensional scaling using GCV
  - Concentration plume modeling and detection

Chernobyl Rain Estimation

- Rain post Chernobyl
  - d=5
  - Dimensional scaling
  - Journal of Geographic Information and Decision Analysis, vol. 2, no. 2, pp. 182 - 193, 1998
- Independent Variables
  - Longitude
  - Latitude
  - Elevation
  - Change in elevation with respect to latitude
  - Change in elevation with respect to longitude
- GCV for scale coefficients – dimensional scaling
  - (x’,y’,z’,s’,t’) = (x, iy, jz, kdz/dx, ldz/dw)

Chernobyl Rain Estimation



Splines on the Sphere

- Legendre polynomials
- Dilogarithms
- Trilogarithms
- R Code
- Evaluate

$$k_m(x) = 1/(4\pi) \sum_{\nu=1}^{\infty} \frac{2\nu+1}{(\nu(\nu+1))^m} P_\nu(x), \quad |x| \leq 1$$

Splines on the Sphere

- Logarithm

$$-\ln(1 - x) = \sum_{\nu=1}^{\infty} x^{\nu}/\nu, \quad -1 \leqslant x < 1$$

- Dilogarithm

$$Li_2(x) = \sum_{\nu=1}^{\infty} x^{\nu}/\nu^2, \quad |x| \leqslant 1$$

- Trilogarithm

$$Li_3 = \sum_{\nu=1}^{\infty} x^{\nu}/\nu^3, \quad |x| \leqslant 1$$

Splines on the Sphere m = 2

$$\sum_{\nu=1}^{\infty} \frac{2\nu+1}{\nu^2(\nu+1)^2} P_\nu(x) P_\nu(z)$$

$$=$$

$$1 - Li_2(1) - \ln(1/2 - x/2)\ln(1/2 + z/2) + Li_2(1/2 + x/2)$$

$$+ Li_2(1/2 - z/2), \quad -1 < x \le z < 1,$$

$$\sum_{\nu=1}^{\infty} \frac{2\nu+1}{\nu^2(\nu+1)^2} P_\nu(x)$$

$$= 1 - \ln(1/2 + x/2)\ln(1/2 - x/2)$$

$$- Li_2(1/2 - x/2), \quad |x| \le 1$$

$$Li_2(1) = \sum_{\nu=1}^{\infty} 1/\nu^2 = \pi^2/6$$

Splines on the Sphere m = 3

$$\sum_{\nu=1}^{\infty} \frac{2\nu+1}{\nu^3(\nu+1)^3} P_\nu(x)\, P_\nu(z)$$

$$= 4\,\mathrm{Li}_3(1) - 2\mathrm{Li}_3(1/2 - x/2) - \mathrm{Li}_3(1/2 + z/2)$$

$$+ \mathrm{Li}_2(1) - \mathrm{Li}_2(1/2 + x/2) - \mathrm{Li}_2(1/2 - z/2)$$

$$+ \ln(1/2 - x/2)[\mathrm{Li}_2(1/2 - x/2) + \mathrm{Li}_2(1/2 - z/2)]$$

$$+ \ln(1/2 + z/2)[\mathrm{Li}_2(1/2 + x/2) + \mathrm{Li}_2(1/2 + z/2)]$$

$$+ \ln(1/2 - x/2)\ln(1/2 + z/2) - 2, \quad -1 < x \leq z < 1$$

$$\sum_{\nu=1}^{\infty} \frac{2\nu+1}{\nu^3(\nu+1)^3} P_\nu(x)$$

$$\mathrm{Li}_3(1) = \sum_{\nu=1}^{\infty} 1/\nu^3 = 1.20205690\ldots$$

$$= -2 + \mathrm{Li}_2(1) + 2\mathrm{Li}_3(1)$$

$$- \mathrm{Li}_2(1/2 + x/2) + \ln(1/2 - x/2)\mathrm{Li}_2(1/2 - x/2)$$

$$- 2\mathrm{Li}_3(1/2 - x/2), \quad -1 < x < 1.$$

ANOVA table

Source	Sum of Squares	Degrees of Freedom
Null Space	$z_\sigma^T Q_1 Q_1^T z_\sigma$	M
Kernel	$w^T D_B{}^2 (D_B + N\lambda I)^{-2} w$	$N_N - \sum_{i=1}^{N_N} N\lambda/(b_i + N\lambda)$
Residual	$w^T[I - D_B{}^2(D_B + N\lambda I)^{-2}]w$	$\sum_{i=1}^{N_N} N\lambda/(b_i + N\lambda)$
Pure Error	$z_\sigma^T Q_2 U_2 U_2^T Q_2^T z_\sigma$	N_0
Total	$z_\sigma^T z_\sigma$	N

Multiple Minima of the GCV

- J. Wendelberger (1987): “Multiple Minima of the Generalized Cross-Validation Function: Paint Attribute Data,” Department of Mathematics, General Motors Research Laboratories Report.

Industry: Spatial Location Modeling

- Statistical consulting in the automotive industry
- Dealer network planning
- Marketing
- Expert witness
- Gravity model of buyer behavior
- Agent based model of buyer behavior
- Expert witness in statistics
- Marketing

Nanoscience and Microsystems Engineering

- Nanoscience engineering
  - 10^{-9} meters
  - The forces at this scale
- Microsystems engineering
  - Clean room
  - Minimal lancing blood glucose detector
- PhD advisors Professor Terry Loring/Susan Atlas
  - The electron cloud/atomic energy levels
  - Topological insulators
  - Disorder and eigen-value distribution
  - Spintronics
  - Majorana fermions

The Nanoscale

Richard P. Feynman 1959 There's plenty of room at the bottom

- Transcript of a talk given on December 26, 1959, at the annual meeting of ;he American Physical Society at the California Institute of Technology
- JOURNAL OF MICROELECTROMECHANICAL SYSTEMS VOL. **I ,** NO. I . MARCH 1992

"At the atomic level, we have new kinds of forces and new kinds of possibilities, new kinds of effects."

Sensitivity of physical quantities to length scale 1 of 2

Physical Quantities	Examples	Governing Equation	Sensitivity to Length Scale
Van der Waals Forces [2] $\breve{A}$:= *Hamaker Constant* A :=*Area* d := *Distance between objects* r :=*Radius* r_i :=*Radius of object "i"* l := *Facing lengths of two objects*	***Case1:*** Two Spheres ***Case 2:*** A sphere and a surface ***Case 3:*** Two Cylinders ***Case 4:*** Two crossed cylinders ***Case 5:*** Two Surfaces	$F = \frac{\breve{A}}{6}\left(\frac{r_1 r_2}{r_1 + r_2}\frac{1}{d^2}\right)$ $F = \frac{A}{6}\left(\frac{r}{d^2}\right)$ $F = -\frac{A}{8\sqrt{2}}\left(\sqrt{\frac{r_1 r_2}{r_1 + r_2}}\frac{l}{\sqrt{d^5}}\right)$ $F = \frac{A}{6}\left(\frac{\sqrt{r_1 r_2}}{d^2}\right)$ $F = \frac{A}{6\pi}\left(\frac{1}{d^3}\right)$	l^{-1} l^{-1} l^{-1} l^{-1} l^{-3}
Viscous forces μ := *Dynamic viscosity* V_0 := *Relative velocity*	***Case 1:*** Two infinite plates ***Case 2:*** Two finite plates	$F = \mu V_0\left(\frac{1}{d}\right)$ $F = \mu V_0\left(\frac{A}{d}\right)$	l^{-1} l^{1}
Electrostatic force ϵ_r := *Relative static permittivity* ϵ_0: =*Vacuum permittivity* V_e :=*Electrical potential* h := *out of plane thickness*	***Case 1:*** Infinite parallel plates capacitor ***Case 2:*** Finite parallel plates at distance d ***Case 3:*** Comb drive [3]	$F = \frac{\epsilon_0 \epsilon_r V_e^2}{2}\left(\frac{1}{d^2}\right)$ $F = \frac{\epsilon_0 \epsilon_r V_e^2}{2}\left(\frac{A}{d^2}\right)$ $F = \frac{\epsilon_0 \epsilon_r V_e^2}{2}\left(\frac{h}{d}\right)$	l^{-2} l^{0} l^{0}
Thermal Expansion E_y :=*Young modulus of elasticity* α_T :=*Therma expansion coefficient* ΔT :=*Temperature change*	***Case 1:*** Constrained column	$F = E_y \alpha_T \Delta T A$	l^{2}
Magnetic forces [4] μ_0 := *Vacuum permeability* d := *Distance between wires* l := *Length along wire* I_i := *Current in wire "i"* A_0 := *Cross sectional area* A_s := *Surface area* $\dot{Q}_s$:= *Surface heat flow rate* I_e := *Electrical current*	***Case 1:*** Constant current density with the boundary condition $\frac{I_e}{A_0} = cons.$ ***Case 2:*** Constant heat flow through the surface of the wire with the boundary condition $\frac{\dot{Q}_s}{A_s} = cons.$ ***Case 3:*** Constant temperature rise of wire with the boundary condition $\Delta T = cons.$	$F = \frac{\mu_0}{2\pi}\frac{l}{d}I_1 I_2$ $F = \frac{\mu_0}{2\pi}\frac{l}{d}I_1 I_2$ $F = \frac{\mu_0}{2\pi}\frac{l}{d}I_1 I_2$	l^{4} l^{3} l^{2}

MEMS and NEMS, UNM NSMS 519, Professor Zayd Leseman

Sensitivity of physical quantities to length scale 2 of 2

Piezoelectric force [5] ϵ := *Mechanical strain* E_e := *Electrical field* e_p := *Piezoelectric Constant* $\frac{\text{Chanrge density}}{\text{applied strain}}$ E_y^E := *Young modulus at constant* E_e	***Case 1:*** 1-D unconstrained actuation	$F = -e_p V\left(\frac{A_0}{d}\right) + E_y^E \epsilon(A_0)$	l^1 & l^2
Drag Force ρ := *Density* C_d := *Drag Coefficient* A_p := *Projected are normal to flow*	***Case 1:*** Infinite cylinder (C_d =.47) ***Case 2:*** Flat plate perpendicular to flow (C_d = 1.28)	$F = \frac{1}{2}\rho V_0^2 C_d(A_p)$	l^2
Surface Tension Force γ := *Surface Tension* p := *Perimeter*	***Case 1:*** Fluid trapped between two circular plates	$F = \gamma(p)$	l^1
Inertia and Weight g := *Gravity* a := *Acceleration*	***Case 1:*** Weight ***Case 2:*** Inertia Force	$F = \rho g(\forall)$ $F = \rho a(\forall)$	l^3 l^3

$\forall$:= *Volume*			
Mass Moment of Inertia ρ_l := *Mass per unit length* ρ_A := *Mass per unit area* ρ_V := *Mass per unit volume* r := *Radius*	***Case 1:*** Sphere ***Case 2:*** Thin circular disk ***Case 3:*** Slender Bar	$\bar{I} = \frac{8\pi}{15}\rho_V(r^5)$ $\bar{I} = \frac{\pi}{2}\rho_A(r^4)$ $I = \frac{1}{12}\rho_l(l^3)$	l^5 l^4 l^3
Shape-Memory Alloy [6] ν := *Poison's ratio* h_f := *Shape memory alloy film thickness* h_s := *Substrate thickness* R_i := *Initial radius of curvature* R_i := *Radius of curvature of the substrate with SAM film*	***Case 1:*** Force caused by shape memory alloy on a substrate	$F = -\frac{E_y}{1-\nu}\left(\frac{A_0 h_s^2(r_1 - r_2)}{6 h_f r_1 r_2}\right)$	l^2

MEMS and NEMS, UNM NSMS 519, Professor Zayd Leseman

The Forces at the Nanoscale

Sensitivity of physical quantities to length scale

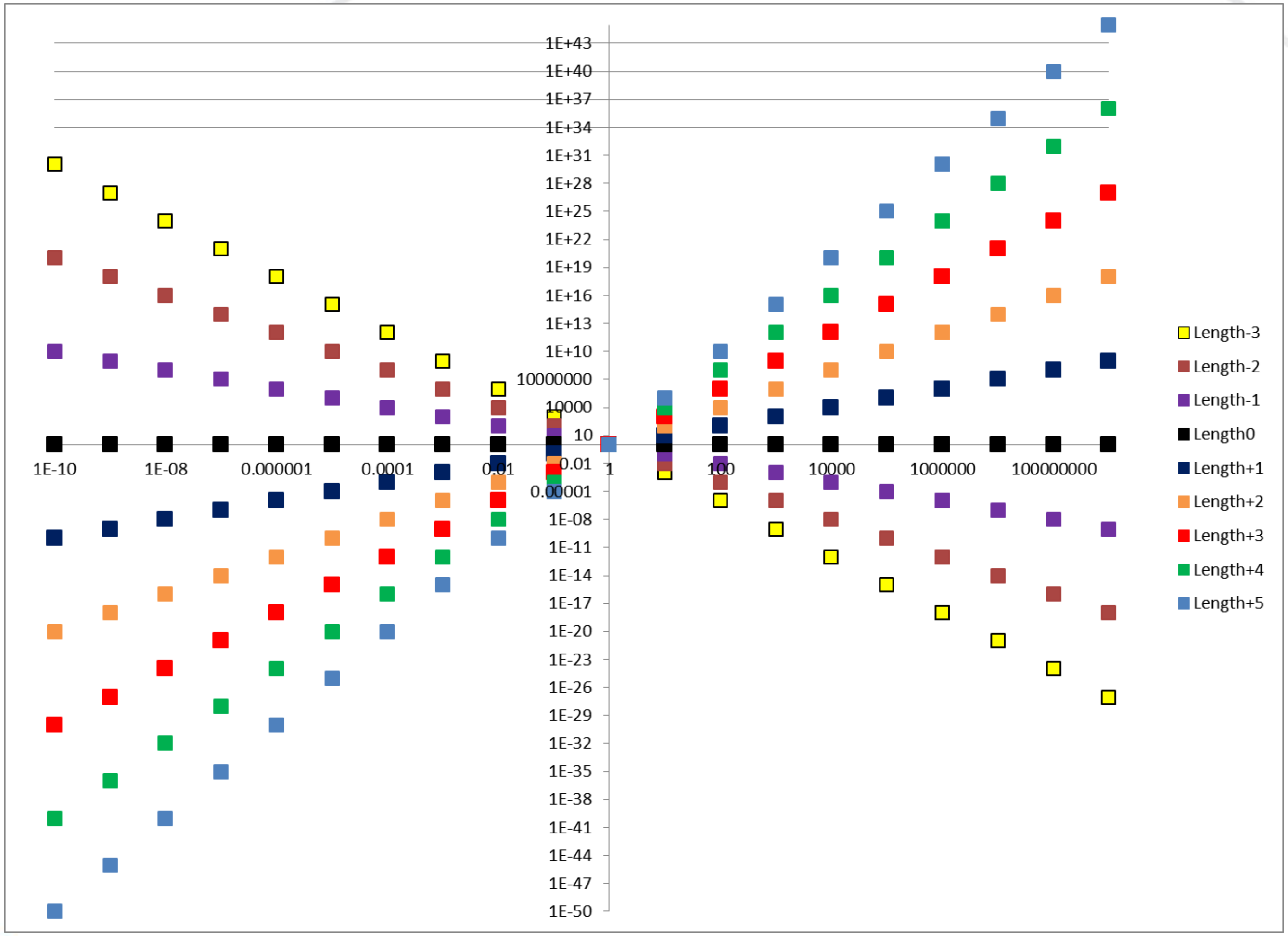
– MEMS and NEMS, UNM NSMS 519, Professor Zayd Leseman

1. Van der Waals – length^{-3} or length^{-1}
2. Viscous – length^{-1} or length^{+1}
3. Electrostatic – length^{-2} or length^{0}
4. Thermal Expansion – length^{+2}
5. Magnetic – length^{+2}, length^{+3} or length^{+4}
6. Piezoelectric – length^{+1} or length^{+2}
7. Drag – length^{+2}
8. Surface Tension – length^{+1}
9. Inertia and Weight – length^{+3}
10. Mass Moment of Inertia – length^{+3}, length^{+4} or length^{+5}
11. Shape memory Alloy – length^{+2}

The Forces at the Nanoscale

Sensitivity of physical quantities to length scale

- MEMS and NEMS, UNM NSMS 519, Professor Zayd Leseman



- Van der Waals – length^{-3} or length^{-1}
- Viscous – length^{-1} or length^{+1}
- Electrostatic – length^{-2} or length^{0}
- Thermal Expansion – length^{+2}
- Magnetic – length^{+2}, length^{+3} or length^{+4}
- Piezoelectric – length^{+1} or length^{+2}
- Drag – length^{+2}
- Surface Tension – length^{+1}
- Inertia and Weight – length^{+3}
- Mass Moment of Inertia – length^{+3}, length^{+4} or length^{+5}
- Shape memory Alloy – length^{+2}

The Schrödinger Equation

Dr. Erwin Schrödinger

- Four Lectures on Wave Mechanics.
- Delivered at the Royal Institution, London, on 5, 7 and 14 March 1928

"Substituting from (12) and (8) in (10) and replacing p by Ψ(…) we obtain"

$$\nabla^2 \Psi + \frac{8\pi^2 m}{h^2}(E - V)\Psi = 0$$

"(…) A simplification in the problem of the "mechanical waves" consists in the absence of boundary conditions. I thought the later simplification fatal when I first attacked these equations. Being insufficiently versed in mathematics, I could not imagine how proper vibration frequencies could appear without boundary conditions. Later on I recognized that the more complicated form of the coefficients (i.e. the appearance of V(x,y,z)) takes charge, so to speak, of what is ordinarily brought about by the boundary conditions, namely, the selection of definite values of E."

Quantum Bayes?

The key ingredient is a hypothetical structure called a "symmetric informationally complete positive-operator-valued measure," or SIC (pronounced "seek") for short. This is a set of d^2 rank-one projection operators $\Pi_i = |\psi_i\rangle\langle\psi_i|$ on a finite d-dimensional Hilbert space such that

$$\left|\langle\psi_i|\psi_j\rangle\right|^2 = \frac{1}{d+1} \quad \text{whenever} \quad i \neq j \; . \tag{3}$$

Because of their extreme symmetry, it turns out that such sets of operators, when they exist, have three very fine-tuned properties: 1) the operators must be linearly independent and span the space of Hermitian operators, 2) there is a sense in which they come as close to an orthonormal basis for operator space as they can (under the constraint that all the elements in a basis be positive semi-definite), and 3) after rescaling, they form a resolution of the identity operator, $I = \sum_i \frac{1}{d}\Pi_i$.

QBism, the Perimeter of Quantum Bayesianism

Christopher Fuchs (2010)

arXiv:1003.5209

Nuclear Material and Accountability

- Material balance
  - Inventory difference
  - Measurement devices

How to measure radioactive materials?

- Weight/mass
- Alpha particles
- Beta particles
- Gamma rays
- Neutron flux
- Chemistry
- Isotopic composition
- Heat

Challenges to measure radioactive materials

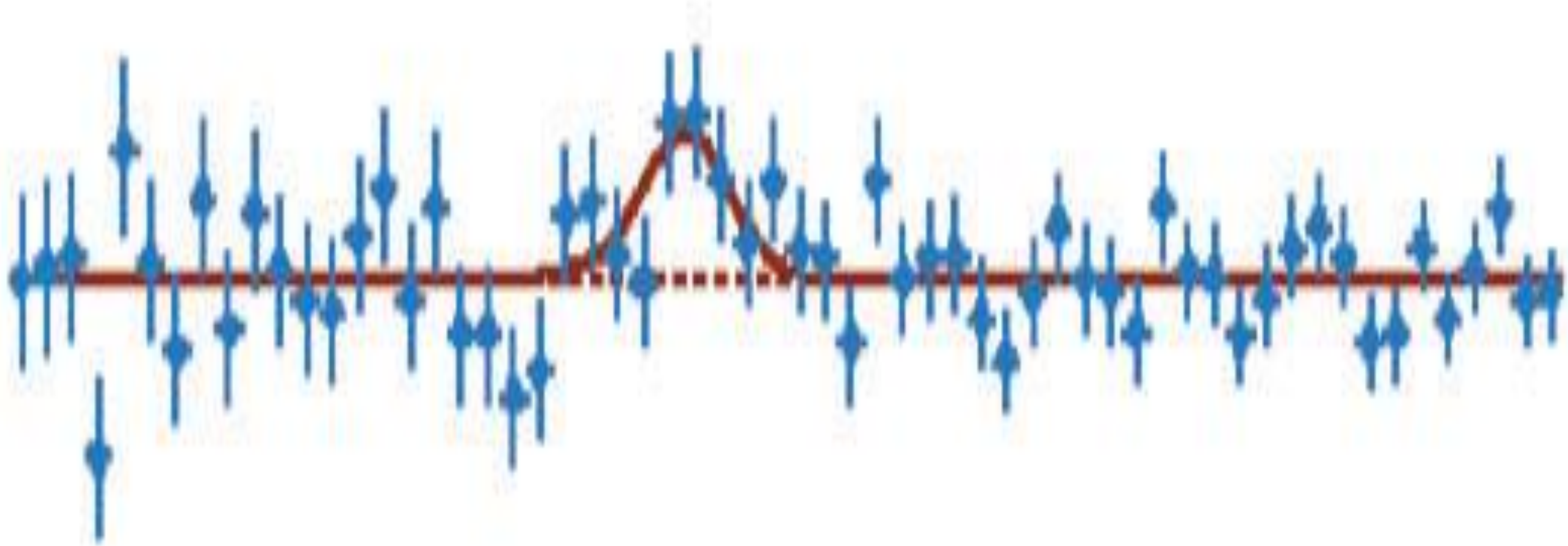
- Health effects
- Accessibility
- Decay
- Conversions
- Self shielding
- Container shielding
- Non-homogeneous
- Isotope distribution

Classical to Quantum Physics

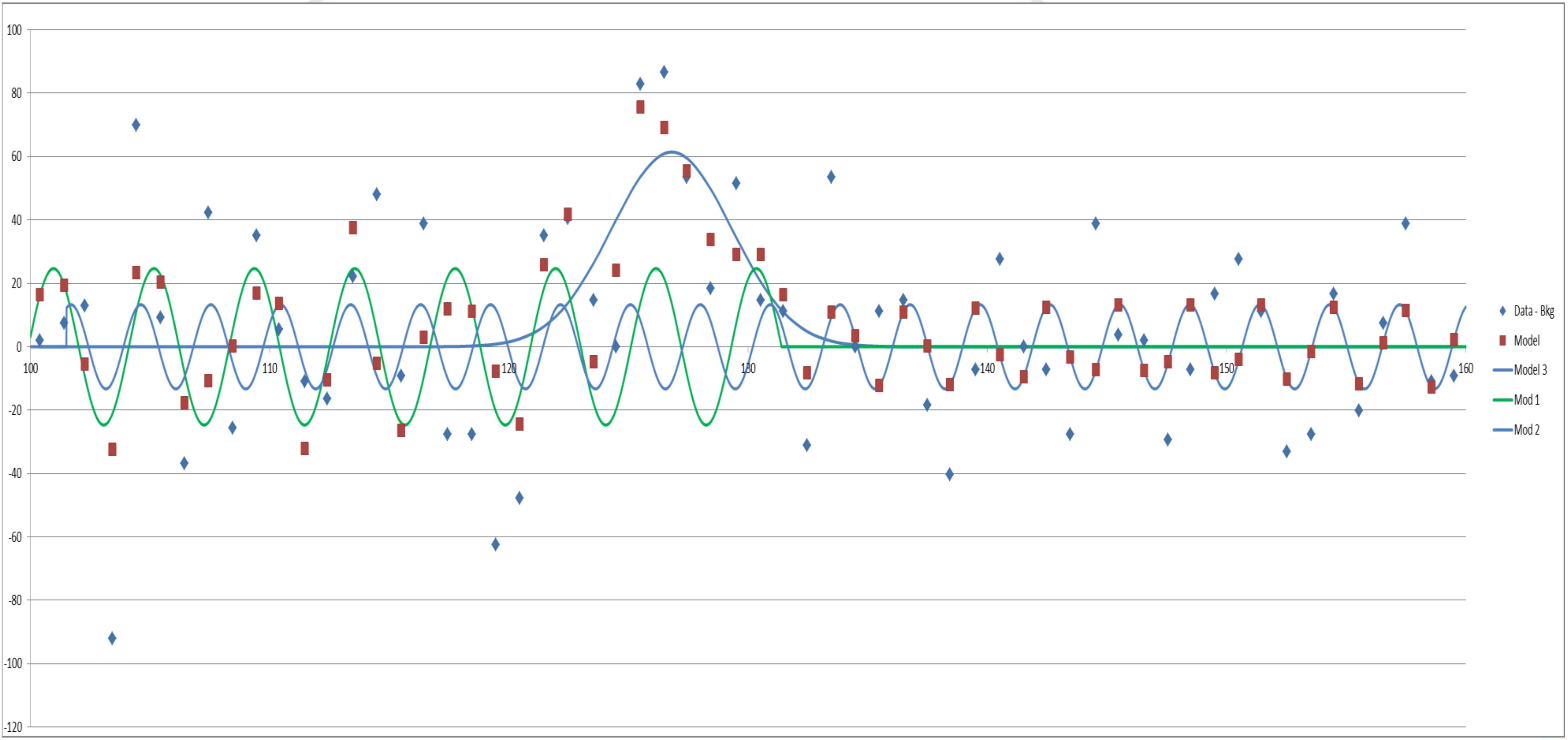
- Waves
- Operators
- Laser cooling
  - Back to the lattice
  - New state of matter
- Equilibrium of processes
  - P.A.M. Dirac
  - A. Einstein

- "The Role of Statistics in the Discovery of the Higgs Boson", David A. van Dyk, Annual Review of Statistics and Its Application, 2014, 1:41-59.

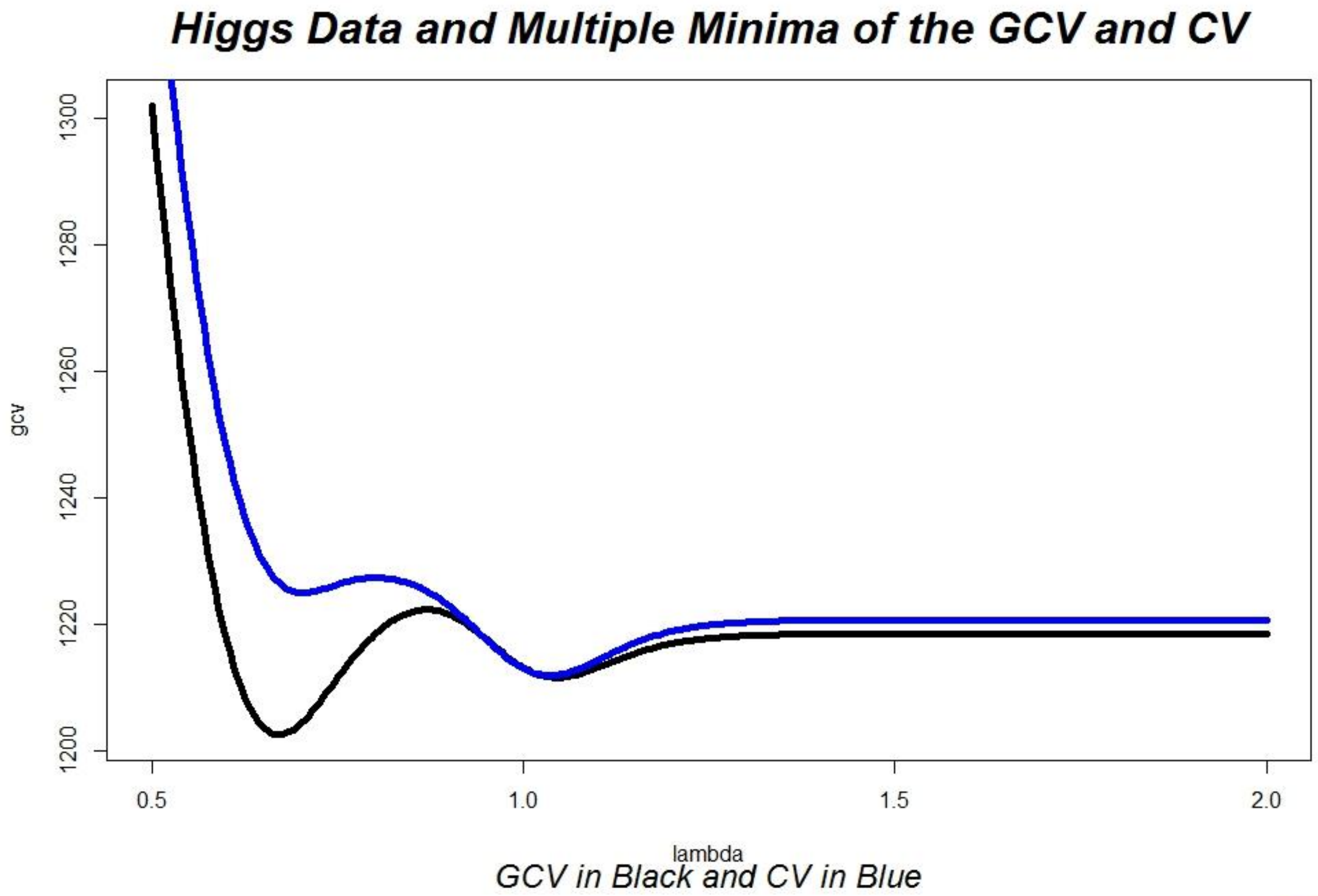
Higgs Boson Detection



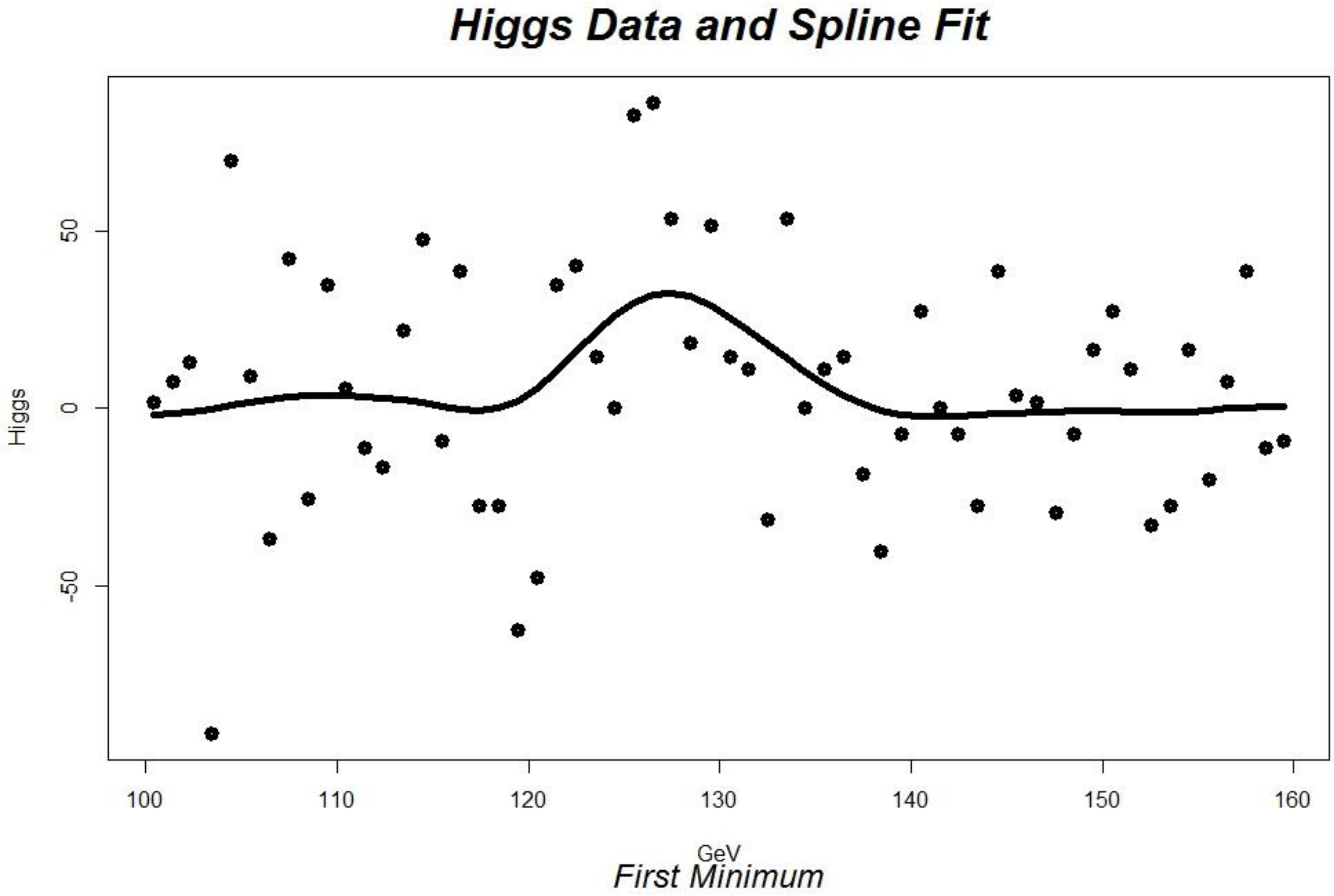
Higgs Boson Detection



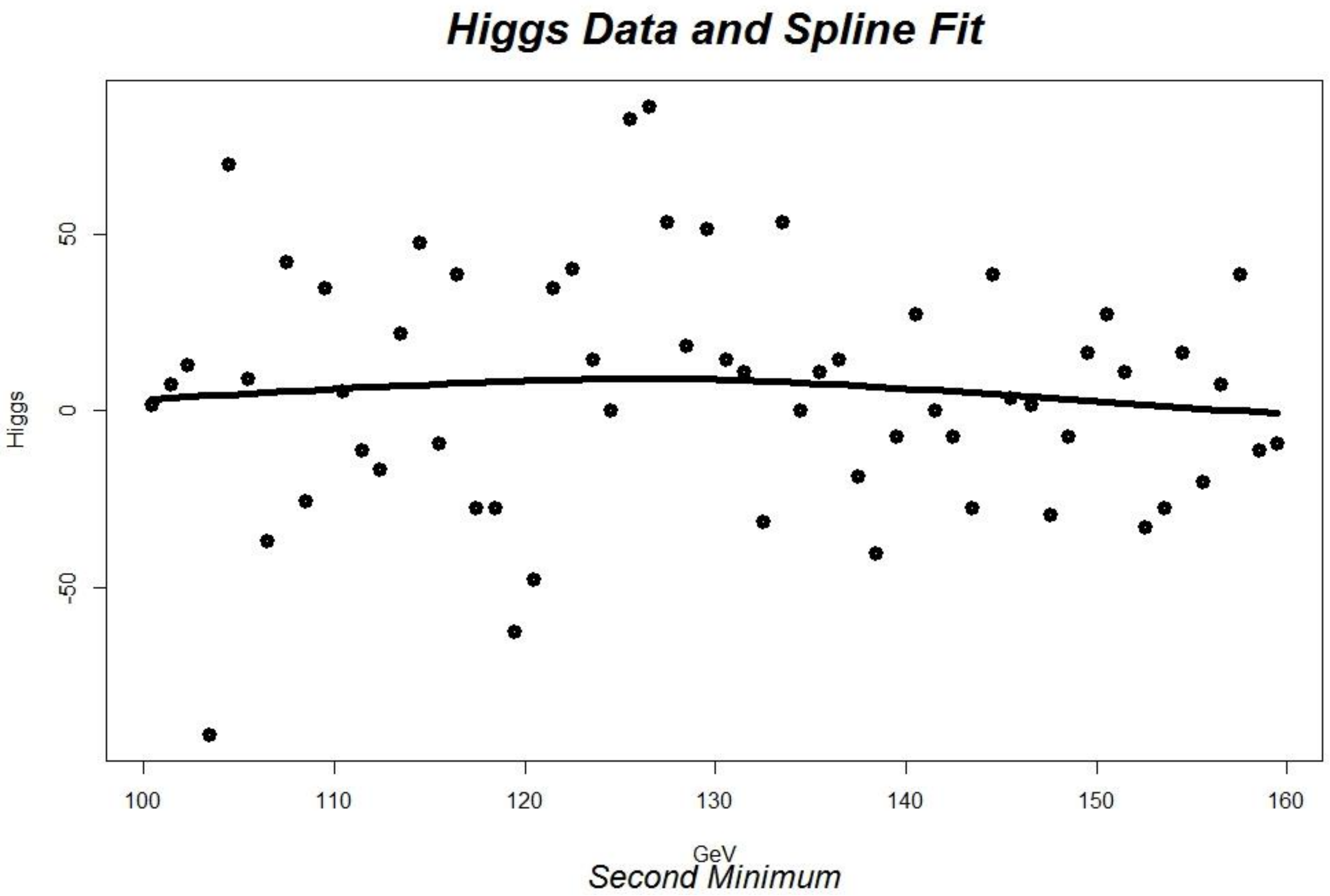
Higgs Boson Multiple Minima



Higgs Boson Multiple Minima



Higgs Boson Multiple Minima



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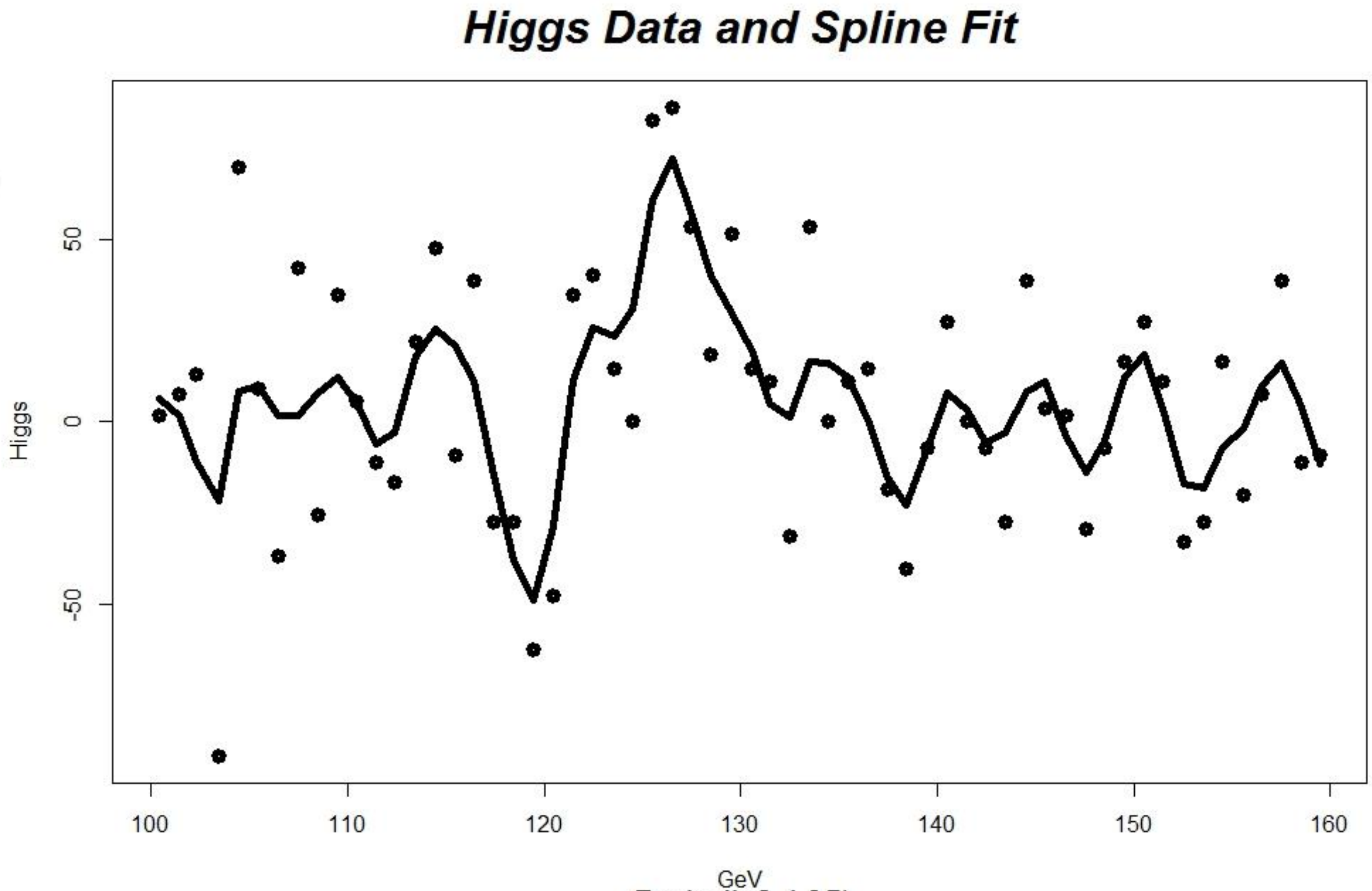
Higgs Boson Multiple Minima



Periodic? (.35)

Higgs Boson Detection

- Utilize linear functional for Gaussian distribution
- Treat as a density function
- Test for periodic versus smooth function
- Is there a discontinuity as a function of energy?
- Estimate function background
- Estimate function signal
- Account for censoring?

Professor Grace Wahba

- An infectious curiosity
- A deep understanding
- A mathematical and scientific rigor
- Applied to problems of practical significance

Thank You Professor Grace Wahba!